

Catalytic Oxidation of CW Agents Using H_2O_2 in Ionic Liquids

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IL Waste Management & Research Center

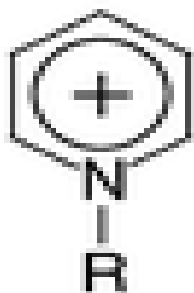
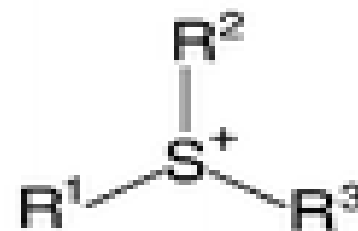
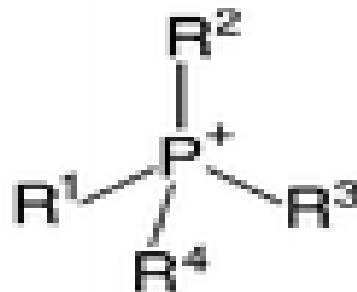
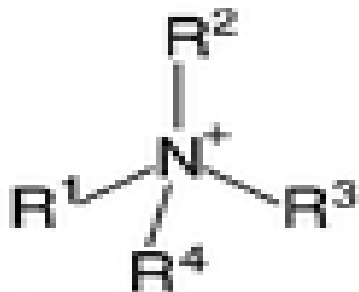
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Structures of ionic liquids

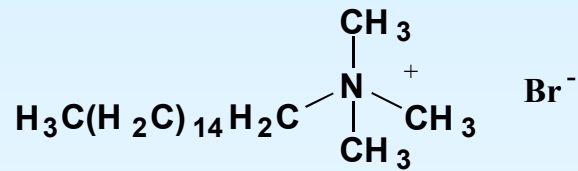
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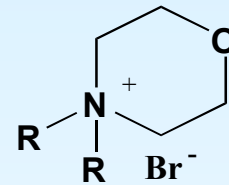
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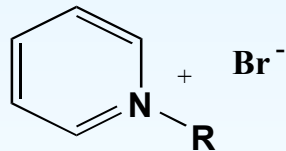
Common Cationic Surfactants



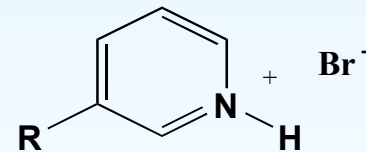
CTAB



morpholinium salts

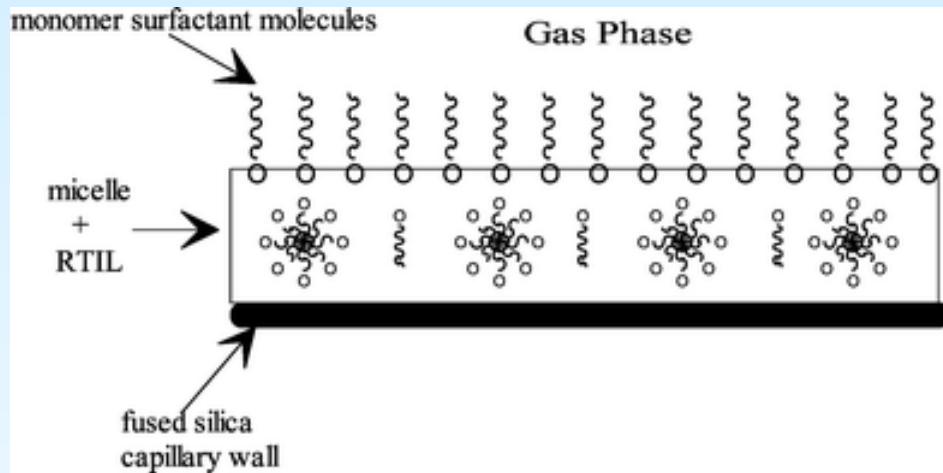


N-alkylpyridinium halides

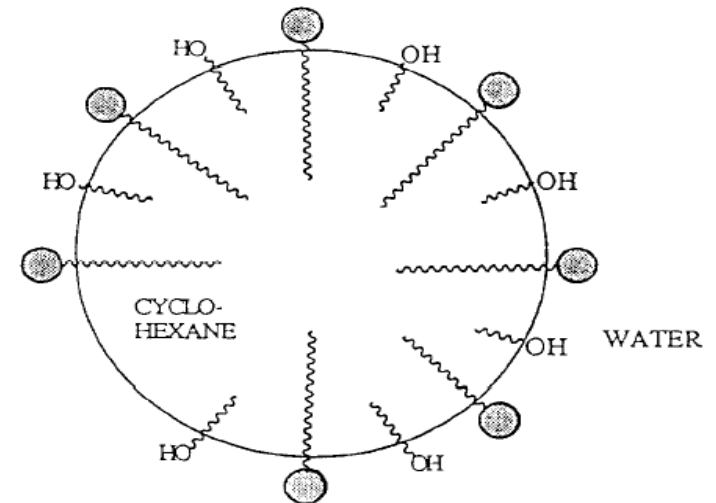


salts of alkyl-substituted pyridine

Micelles to Microemulsions



***Rapid, Cheap
Selective***

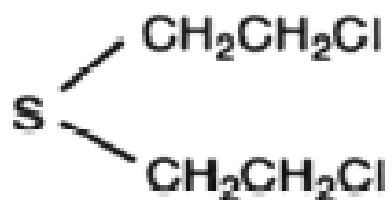


Microemulsion Formulations

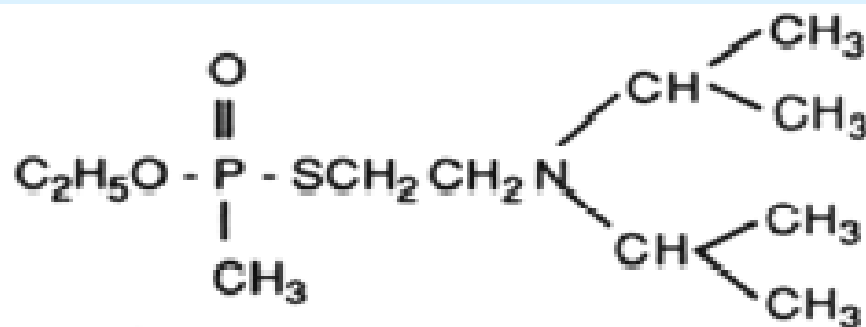
- ◆ *69% H₂O*
- ◆ *9% EtOH*
- ◆ *11% [BMIM] BF₄*
- ◆ *11% Cyclohexane*
o/w

- ◆ *5% H₂O*
- ◆ *10% EtOH*
- ◆ *5% [BMIM] PF₆*
- ◆ *80% Cyclohexane*
w/o

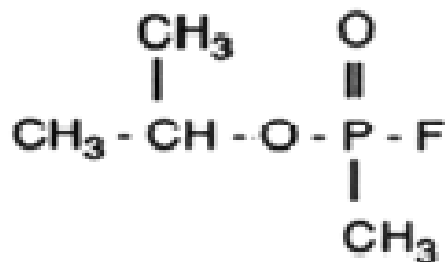
Structures of HD, VX, GB, and GD



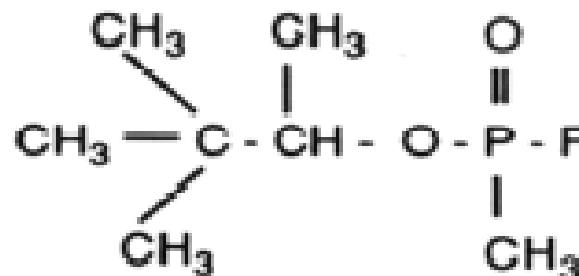
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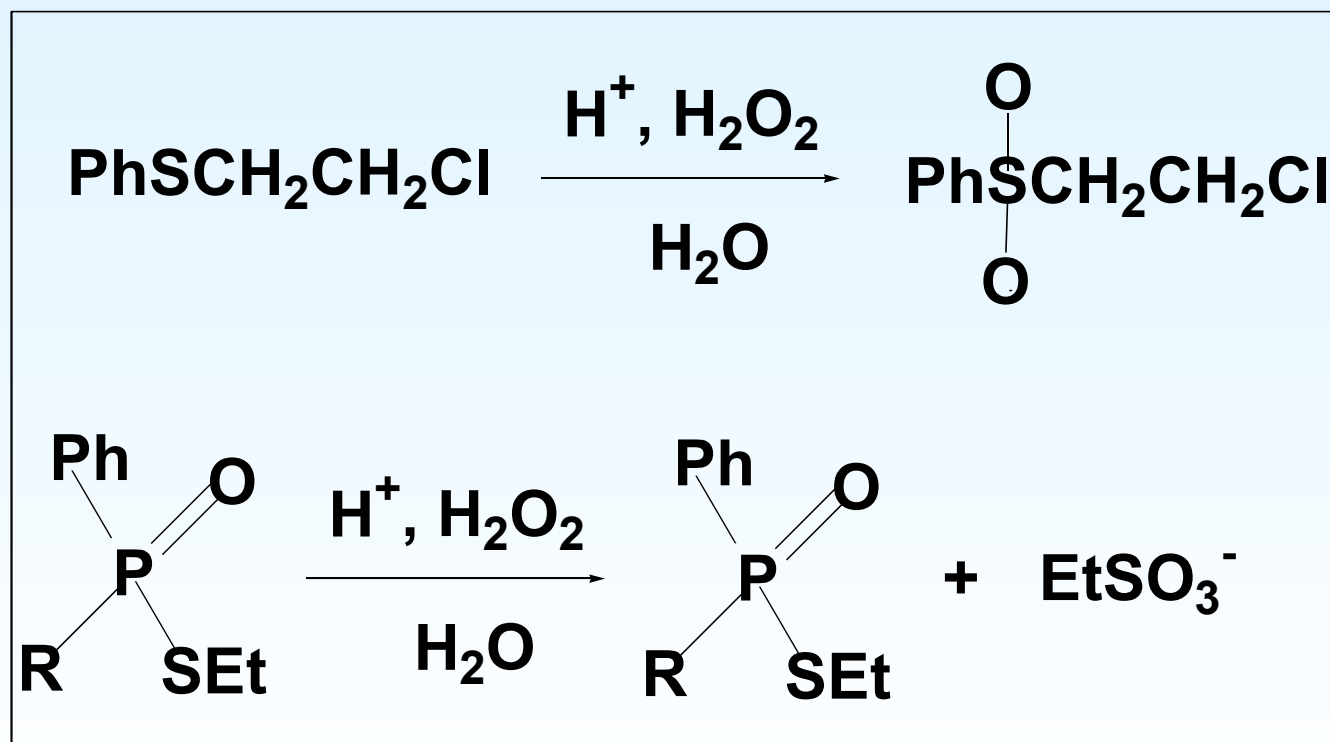
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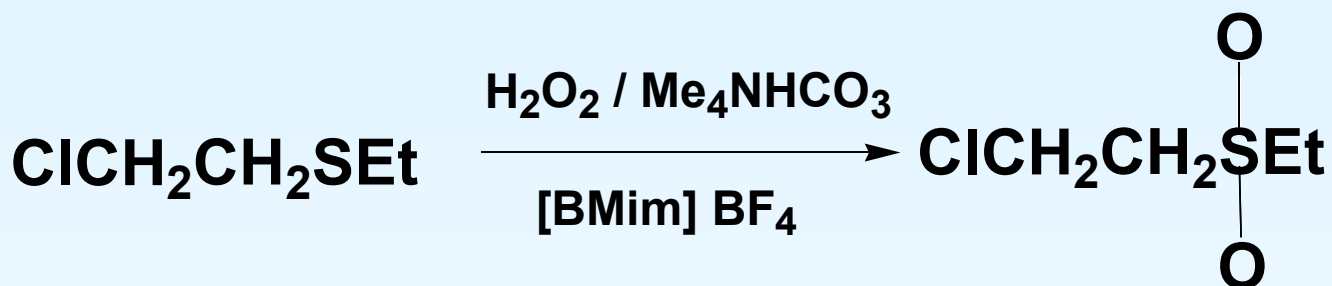
4

(1) HD, mustard; (2) VX; (3) GB or Sarin; (4) GD or Soman

Decontamination of Mustard and Phosphorous (V) Esters



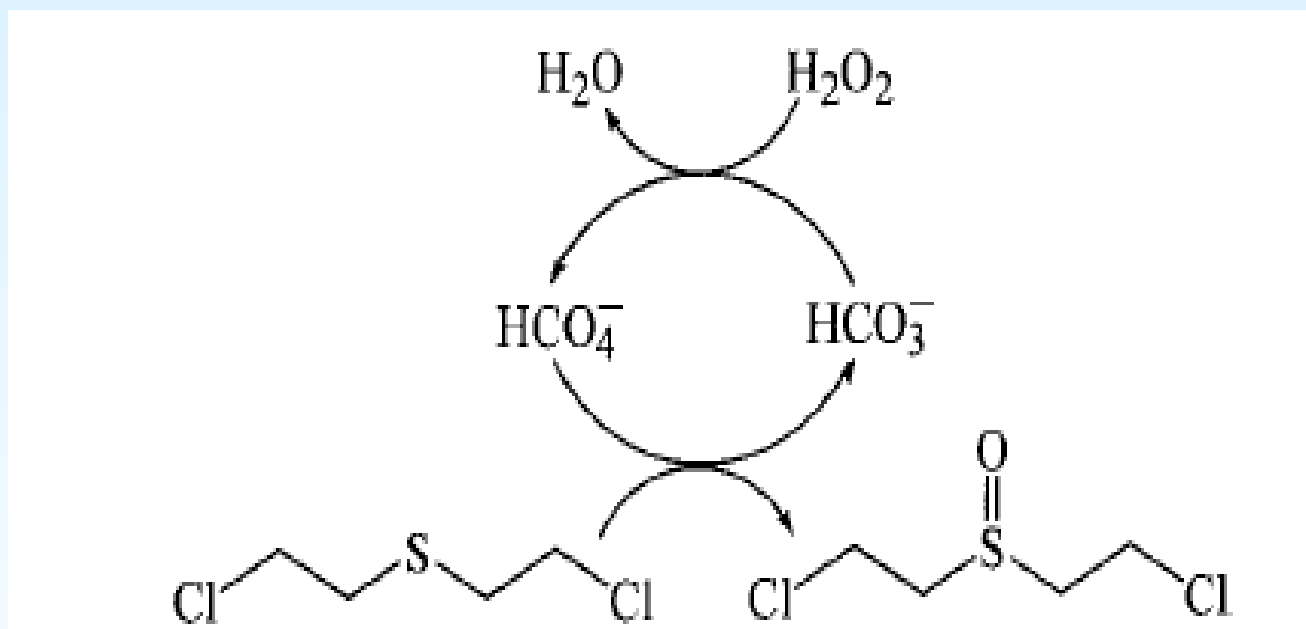
Hydrogen Peroxide with added carbonate



- ◆ *Less than 2 minutes*
- ◆ *2 mole equiv. Of H_2O_2*

Comp (EtOH): Marques et al, J. Org. Chem. 2001, 66, 7588-7595

Hydrogen peroxide, bicarbonate, and organic cosolvents afford rapid, decontamination of CWA

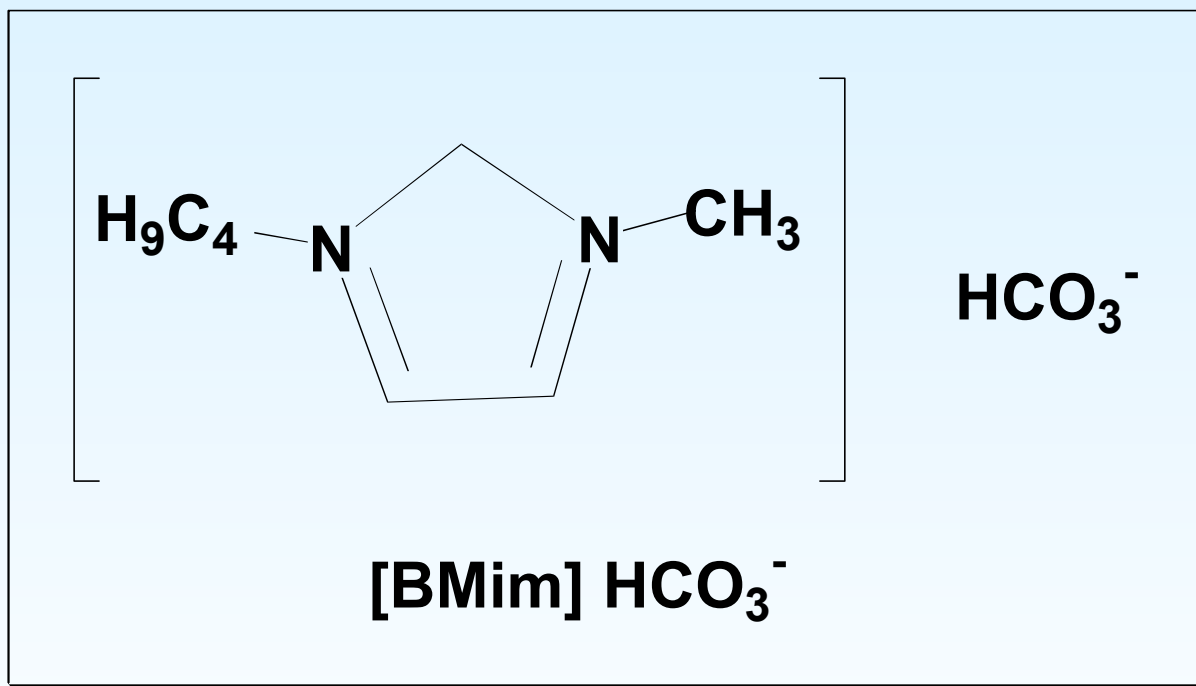


Wagner, G. W.; Yang, Y.-C. *Ind. Eng. Chem. Res.* 2002, 41, 1925 -1928

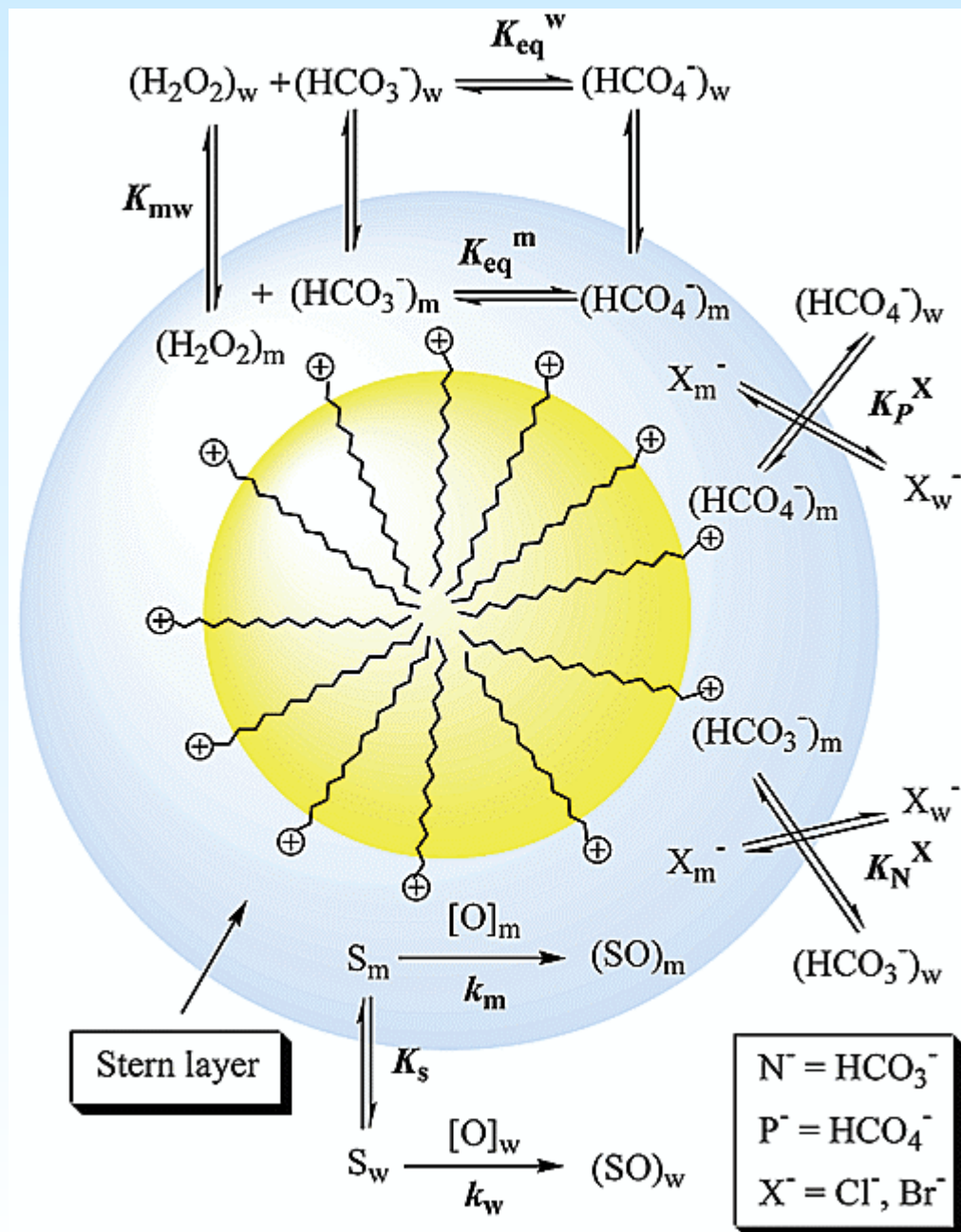
Solubility in a Microemulsion vs glycol/water

<u>solubilizate</u>	<u>microemulsion</u>	<u>3:1 PG/water</u>
paraoxon	470 mg/0.5 mL	215 mg/0.5 mL
half-mustard	75 mg/0.5 mL	b

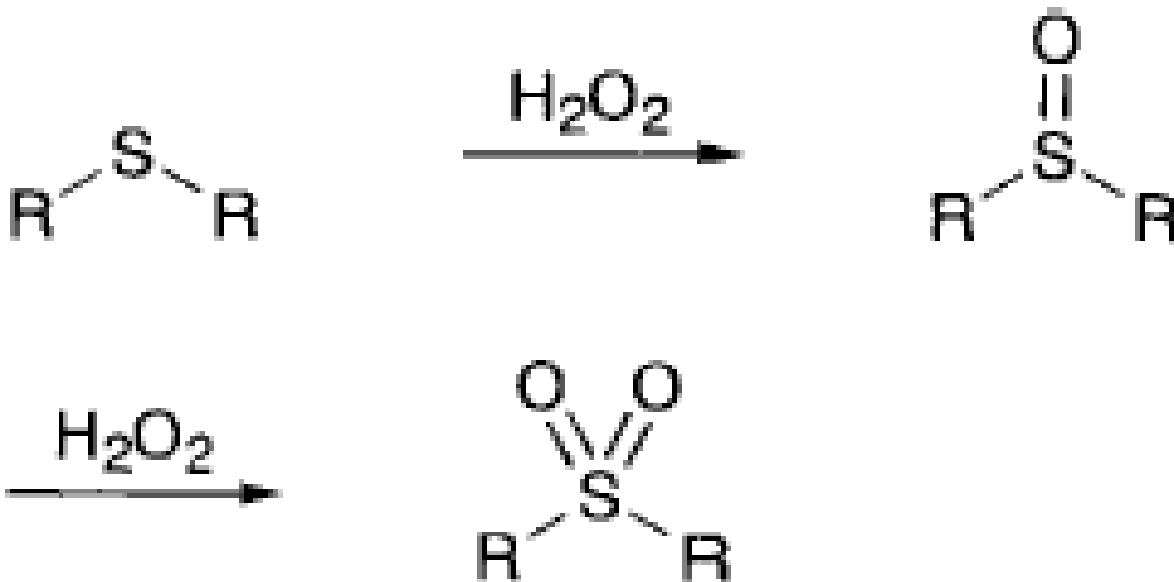
Bicarbonate-activated Peroxide (BAP)



BAP oxidations in aqueous cationic micelles

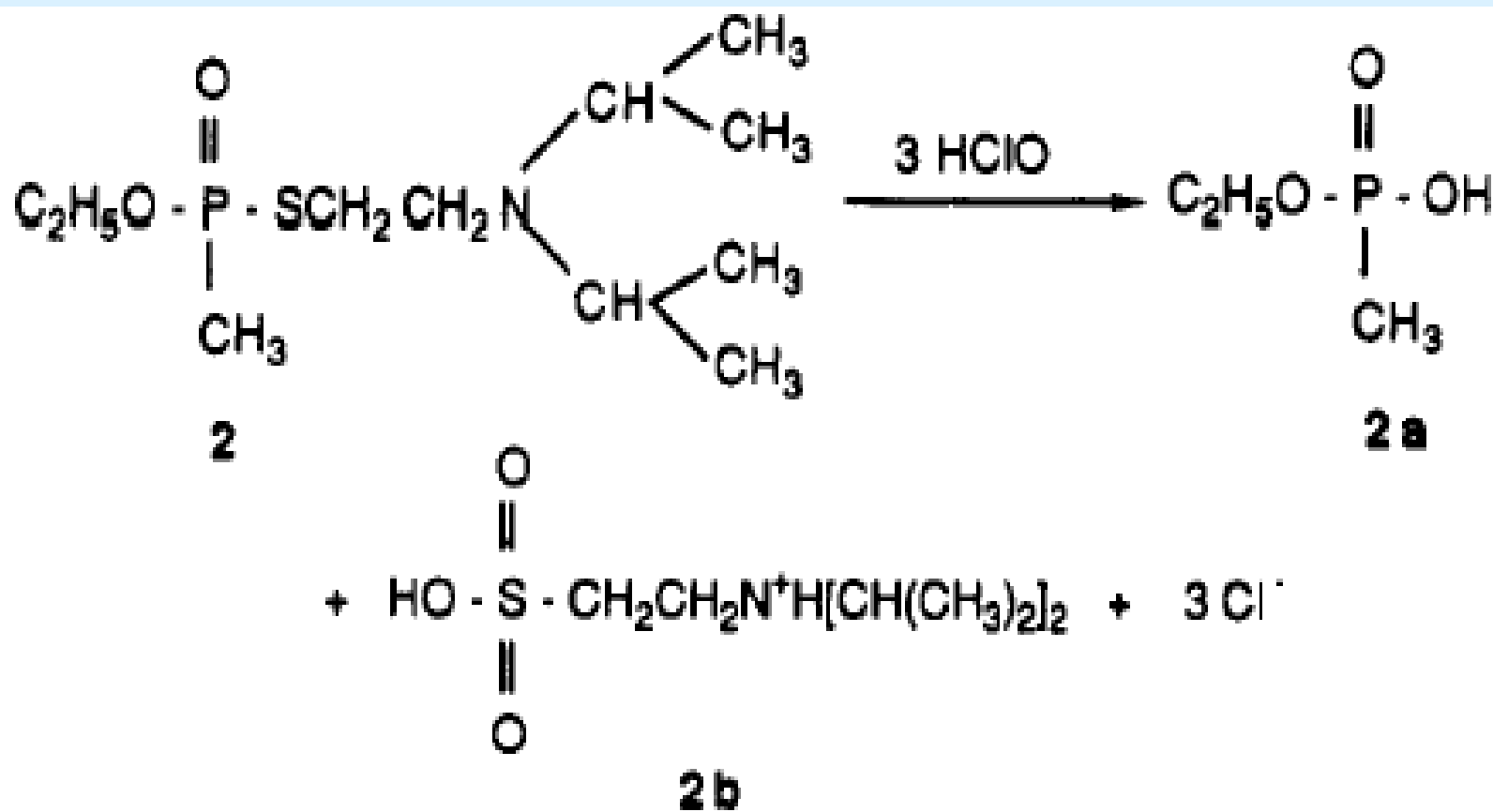


Oxidation of sulfides to sulfoxides and sulfones with 30% H_2O_2



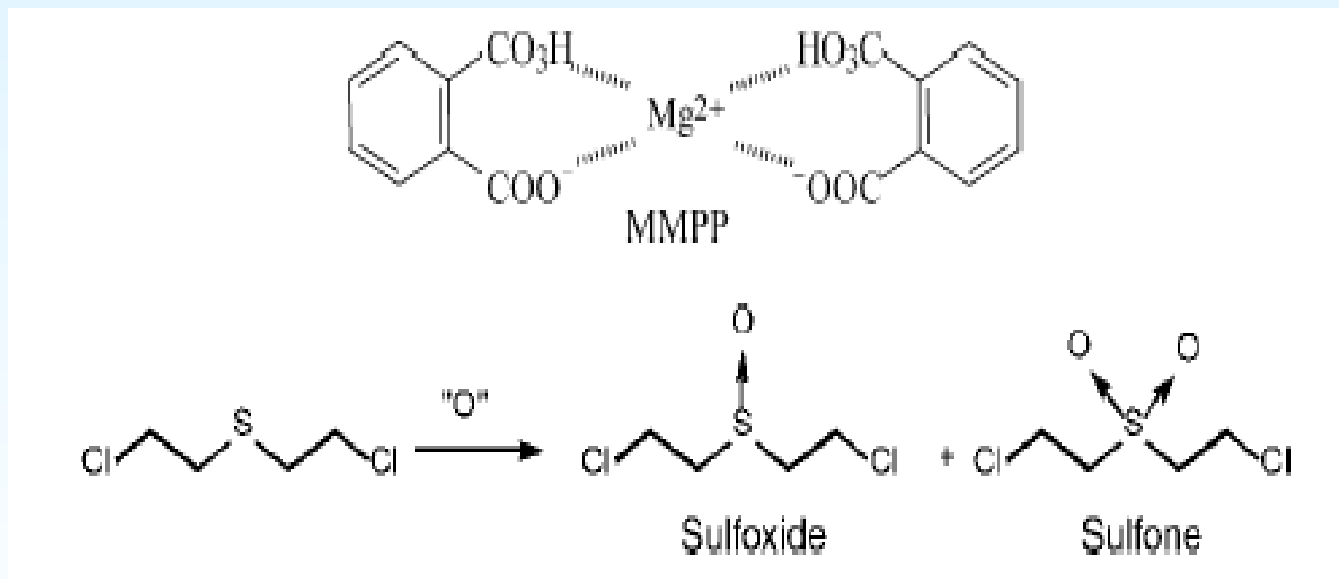
Sato, K. et al *Tetrahedron* 2001, 57, 2469-2476

VX Decontamination by Bleach



Yang, Y.-C. et al. *Chem. Rev.* 1992, 92, 1729-1743

Rapid detoxification of HD using magnesium monoperoxyphthalate (MMPP)



Gonzaga, F. et al., *New Journal of Chemistry* **2001**,
25, 151-155

Mustard oxidation in the microemulsion

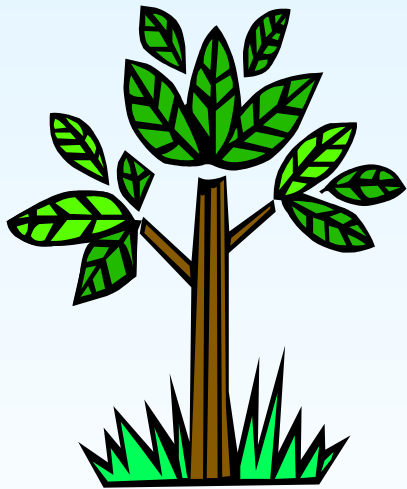
- ◆ **Reaction capacity is excellent**
- ◆ **Sulfoxide is formed quantitatively**
- ◆ **Microemulsions prepared from anionic, non-ionic, and cationic surfactants**

Acknowledgements

***This research is being
Funded by the Army
Research Office (ARO)***

Wisdom on the journey...

*He who can no longer
pause to wonder and
stand rapt in awe is as
good as dead; his eyes
are closed.*



Albert Einstein